

Full wwPDB X-ray Structure Validation Report (i)

Apr 18, 2024 – 11:46 AM EDT

PDB ID : 7H2X

Title: Group deposition for crystallographic fragment screening of Coxsackievirus

A16 (G-10) 2A protease – Crystal structure of Coxsackievirus A16 (G-10) 2A

protease in complex with Z384361454 (A71EV2A-x0207)

Authors: Lithgo, R.M.; Fairhead, M.; Koekemoer, L.; Balcomb, B.H.; Capkin, E.; Chan-

dran, A.V.; Golding, M.; Godoy, A.S.; Aschenbrenner, J.C.; Marples, P.G.; Ni, X.; Thompson, W.; Tomlinson, C.W.E.; Wild, C.; Winokan, M.; Xavier, M.-

A.E.; Fearon, D.; von Delft, F.

Deposited on : 2024-04-04

Resolution : 1.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

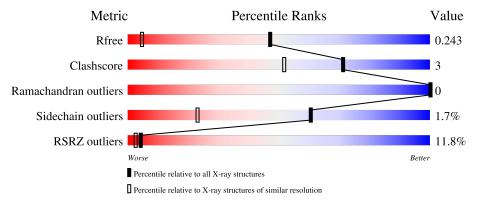
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	A	150	5% 85%	8% • 7%
1	В	150	83%	10% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.36.1



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMS	A	203	-	-	-	X



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2609 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Protease 2A.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	140	Total	С	N	О	S	0	3	0
1	1 A	140	1101	685	196	213	7	U		
1	B	140	Total	С	N	О	S	0	1	0
1	Ъ	140	1089	679	194	209	7			

There are 12 discrepancies between the modelled and reference sequences:

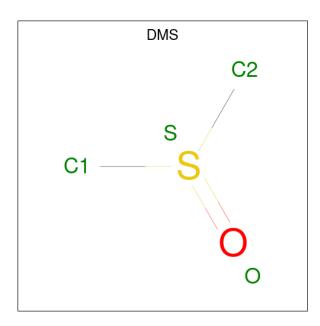
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLN	-	expression tag	UNP Q65900
A	2	GLU	-	expression tag	UNP Q65900
A	3	GLN	-	expression tag	UNP Q65900
A	4	THR	_	expression tag	UNP Q65900
A	5	GLY	-	expression tag	UNP Q65900
A	6	GLY	-	expression tag	UNP Q65900
В	1	GLN	-	expression tag	UNP Q65900
В	2	GLU	-	expression tag	UNP Q65900
В	3	GLN	-	expression tag	UNP Q65900
В	4	THR	-	expression tag	UNP Q65900
В	5	GLY	-	expression tag	UNP Q65900
В	6	GLY	-	expression tag	UNP Q65900

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0

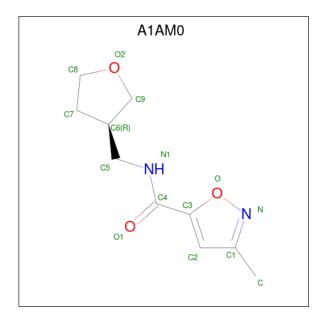
• Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 4				0	0
3	A	1	Total 4	C 2		S 1	0	0
3	В	1	Total 4	C 2	O 1	S 1	0	0

 $\bullet \ \, \text{Molecule 4 is 3-methyl-N-} \\ \{[(3R)\text{-oxolan-3-yl}]\text{methyl}\}\text{-1,2-oxazole-5-carboxamide (three-letter code: A1AM0) (formula: $C_{10}H_{14}N_2O_3$). }$





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
1	D	1	Total	С	N	О	0	0
4	Б	1	15	10	2	3	U	0

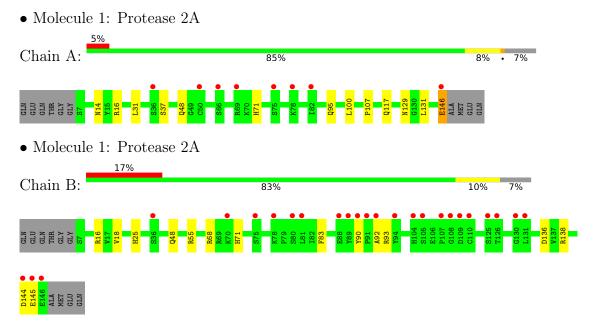
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	199	Total O 199 199	0	0
5	В	191	Total O 191 191	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	86.36Å 56.60Å 64.62Å	Donogitor	
a, b, c, α , β , γ	90.00° 94.67° 90.00°	Depositor	
Resolution (Å)	47.34 - 1.25	Depositor	
Resolution (A)	47.29 - 1.25	EDS	
% Data completeness	99.2 (47.34-1.25)	Depositor	
(in resolution range)	99.3 (47.29-1.25)	EDS	
R_{merge}	0.07	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.12 (at 1.25Å)	Xtriage	
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor	
D D.	0.200 , 0.233	Depositor	
R, R_{free}	0.217 , 0.243	DCC	
R_{free} test set	4104 reflections (4.82%)	wwPDB-VP	
Wilson B-factor (Å ²)	18.4	Xtriage	
Anisotropy	0.042	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 37.9	EDS	
L-test for twinning ²	$ < L > = 0.52, < L^2 > = 0.35$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.96	EDS	
Total number of atoms	2609	wwPDB-VP	
Average B, all atoms (Å ²)	23.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 76.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0880e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, ZN, A1AM0

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bo	nd angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.81	0/1127	0.96	2/1532 (0.1%)
1	В	0.81	0/1115	1.01	3/1516 (0.2%)
All	All	0.81	0/2242	0.98	5/3048 (0.2%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	68	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	В	136	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	A	16	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	16	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	В	138	ARG	NE-CZ-NH1	-5.22	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1101	0	1035	8	0
1	В	1089	0	1027	8	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	12	0	0
3	В	4	0	6	0	0
4	В	15	0	0	0	0
5	A	199	0	0	4	2
5	В	191	0	0	3	2
All	All	2609	0	2080	15	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:83:PHE:CZ	1:B:92:ALA:HB1	2.29	0.67
1:A:117:GLN:HG2	5:A:314:HOH:O	1.93	0.67
1:B:48:GLN:HB3	5:B:361:HOH:O	2.03	0.58
1:A:117:GLN:CG	5:A:314:HOH:O	2.49	0.57
1:A:71:HIS:HD2	5:A:460:HOH:O	1.89	0.55
1:B:55:ARG:HH21	1:B:144:ASP:CG	2.10	0.54
1:B:71:HIS:HE1	5:B:436:HOH:O	1.91	0.54
1:A:100:LEU:HD13	1:A:131:LEU:HD13	1.90	0.53
1:A:14:ASN:ND2	1:A:48:GLN:OE1	2.43	0.51
1:B:90:TYR:CD1	1:B:93:ARG:NH1	2.84	0.46
1:A:31:LEU:HD23	1:B:71:HIS:CD2	2.50	0.45
1:A:37:SER:O	1:A:95:GLN:HG3	2.16	0.45
1:B:25:HIS:CD2	5:B:304:HOH:O	2.70	0.44
1:A:146:GLU:HB3	5:A:336:HOH:O	2.18	0.42
1:B:16:ARG:CZ	1:B:18:VAL:HG11	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
5:A:384:HOH:O	5:B:455:HOH:O[1_545]	1.50	0.70
5:A:463:HOH:O	5:B:450:HOH:O[1_545]	2.08	0.12



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	A	141/150 (94%)	139 (99%)	2 (1%)	0	100	100
1	В	139/150~(93%)	135 (97%)	4 (3%)	0	100	100
All	All	280/300 (93%)	274 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Rotameric Outliers	
1	A	120/124 (97%)	117 (98%)	3 (2%)	47 9
1	В	118/124 (95%)	117 (99%)	1 (1%)	81 53
All	All	$238/248 \ (96\%)$	234 (98%)	4 (2%)	60 23

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	PRO
1	A	129	ASN
1	A	146	GLU
1	В	145	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	71	HIS
1	A	129	ASN
1	В	71	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Type Chain	Chain	Res	Link	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	DMS	A	203	-	3,3,3	0.24	0	3,3,3	0.07	0	
4	A1AM0	В	201	-	13,16,16	0.64	0	12,21,21	0.46	0	
3	DMS	A	202	-	3,3,3	0.46	0	3,3,3	0.20	0	
3	DMS	В	203	-	3,3,3	0.29	0	3,3,3	0.07	0	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1AM0	В	201	-	-	4/6/16/16	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	201	A1AM0	N1-C5-C6-C9
4	В	201	A1AM0	C3-C4-N1-C5
4	В	201	A1AM0	O1-C4-N1-C5
4	В	201	A1AM0	N1-C5-C6-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	140/150 (93%)	0.19	8 (5%) 23 18	12, 19, 30, 60	6 (4%)
1	В	140/150 (93%)	0.62	25 (17%) 1 0	12, 19, 38, 59	23 (16%)
All	All	280/300 (93%)	0.41	33 (11%) 4 2	12, 19, 36, 60	29 (10%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	81	LEU	12.1	
1	A	82	ILE	11.9	
1	A	36[A]	SER	6.7	
1	В	75[A]	SER	6.6	
1	A	75[A]	SER	6.4	
1	A	50	CYS	6.2	
1	В	80	SER	6.1	
1	A	66[A]	SER	6.0	
1	В	110	CYS	5.9	
1	В	36	SER	5.9	
1	В	78	LYS	5.0	
1	В	144	ASP	4.5	
1	В	70	LYS	4.5	
1	A	69	ARG	4.4	
1	A	146	GLU	4.4	
1	В	94	TYR	4.4	
1	В	90	TYR	4.3	
1	В	146	GLU	3.8	
1	В	108	GLY	3.8	
1	В	131	LEU	3.7	
1	A	78	LYS	3.7	
1	В	145	GLU	3.6	
1	В	89	TYR	3.2	
1	В	104	HIS	3.2	

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	В	130	GLY	3.1
1	В	126	THR	3.1
1	В	88	GLU	2.8
1	В	105	SER	2.8
1	В	125	SER	2.5
1	В	109	ASP	2.5
1	В	92	ALA	2.2
1	В	91	PRO	2.1
1	В	107	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ m \AA}^2)$	Q<0.9
3	DMS	A	203	4/4	0.27	0.46	55,57,57,59	4
4	A1AM0	В	201	15/15	0.78	0.17	22,26,43,45	15
3	DMS	В	203	4/4	0.88	0.16	43,46,48,51	0
3	DMS	A	202	4/4	0.95	0.16	30,35,37,39	0
2	ZN	В	202	1/1	0.96	0.05	19,19,19,19	0
2	ZN	A	201	1/1	0.99	0.05	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.

